Construction of QMC Finite Element Methods for Elliptic PDEs with Random Coefficients

SFB Kooperations-Workshop (virtual)

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Joint work with Lukas Herrmann and Peter Kritzer
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Problem statement

Problem setting

Consider the parametric elliptic Dirichlet problem given by

$$\begin{aligned} -\nabla \cdot (a(\boldsymbol{x}, \boldsymbol{y}) \nabla u(\boldsymbol{x}, \boldsymbol{y})) &= f(\boldsymbol{x}) \quad \text{for } \boldsymbol{x} \in D \subset \mathbb{R}^d, \\ u(\boldsymbol{x}, \boldsymbol{y}) &= 0 \qquad\quad \text{for } \boldsymbol{x} \text{ on } \partial D, \end{aligned}$$

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Assumptions:

- gradients are taken w.r.t. $\boldsymbol{x}$ and we assume $f : D \to \mathbb{R}$ lies in $L^2(D)$
- the stochastic variable $\boldsymbol{y} = (y_j)_{j\geq 1}$ is uniformly distributed on $U = \left[-\frac{1}{2}, \frac{1}{2}\right]^{\mathbb{N}}$ with uniform product measure $\mu(\mathrm{d}\boldsymbol{y}) = \bigotimes_{j\geq 1} \mathrm{d}y_j$
- the parametric diffusion coefficient $a(\boldsymbol{x}, \boldsymbol{y})$ depends on the y_j via:

$$a(\boldsymbol{x}, \boldsymbol{y}) = a_0(\boldsymbol{x}) + \sum_{j\geq 1} y_j \, \psi_j(\boldsymbol{x})$$

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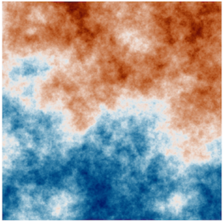
Alternatively: $a(\boldsymbol{x}, \boldsymbol{y}) = \exp(Z(\boldsymbol{x}, \boldsymbol{y}))$ with

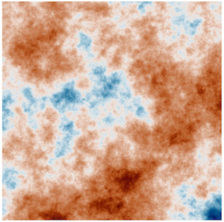
$$Z(\boldsymbol{x}, \boldsymbol{y}) = \sum_{j \geq 1} y_j \, \psi_j(\boldsymbol{x}) \text{ and } y_j \sim \mathcal{N}(0, 1)$$

Illustration of the random field $a(x, y)$

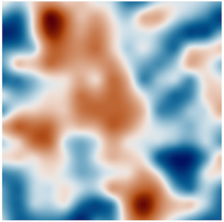
Different realizations[1] of the random field $a(\boldsymbol{x}, \boldsymbol{y})$



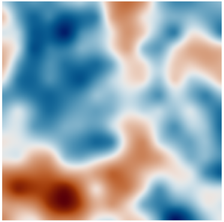
(a) rough random field sample



(b) rough random field sample



(c) smooth random field sample (Matérn kernel)



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[1] By courtesy of Pieterjan Robbe

Solutions of the PDE

Consider the Sobolev space $V = H_0^1(D)$ of functions which vanish on the boundary ∂D with norm

$$\|v\|_V := \left(\int_D \sum_{j=1}^{d} |\partial_{x_j} v(\boldsymbol{x})|^2 \,\mathrm{d}\boldsymbol{x} \right)^{\frac{1}{2}} = \|\nabla v\|_{L^2(D)}.$$

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Variational formulation of PDE

For given $f \in V^*$ and $\boldsymbol{y} \in U$, find $u(\cdot, \boldsymbol{y}) \in V$ such that

$$A(\boldsymbol{y}; u(\cdot, \boldsymbol{y}), v) = \langle f, v \rangle_{V^* \times V} = \int_D f(\boldsymbol{x}) v(\boldsymbol{x}) \,\mathrm{d}\boldsymbol{x} \quad \text{for all} \quad v \in V,$$

with parametric bilinear form $A : U \times V \times V \to \mathbb{R}$ given by

$$A(\boldsymbol{y}; w, v) := \int_D a(\boldsymbol{x}, \boldsymbol{y}) \, \nabla w(\boldsymbol{x}) \cdot \nabla v(\boldsymbol{x}) \,\mathrm{d}\boldsymbol{x} \quad \text{for} \quad w, v \in V.$$

Quantity of interest

Goal: For a bounded linear functional $G \in V^*$, we want to approximate

$$\mathbb{E}[G(u)] := \lim_{s\to\infty} \int_{[-\frac{1}{2},\frac{1}{2}]^s} G(u(\cdot,(y_1,\ldots,y_s,0,0,\ldots)))\,\mathrm{d}y_1\cdots\mathrm{d}y_s$$

by randomized rank-1 lattice rules (or other QMC rules) of the form

$$Q_N(G(u_h^s),\boldsymbol{z},\boldsymbol{\Delta}) = \frac{1}{N}\sum_{k=0}^{N-1} G\left(u_h^s\left(\cdot\,,\left\{\frac{k\boldsymbol{z}}{N}+\boldsymbol{\Delta}\right\}-\left(\frac{1}{2},\ldots,\frac{1}{2}\right)\right)\right)$$

with generating vector $\boldsymbol{z}$ constructed by a CBC-type algorithm and uniform random shift vector $\boldsymbol{\Delta} \in [0,1]^s$.

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• This problem has been extensively studied, see, e.g., Kuo, Schwab, Sloan (2012) or for a broader review article, see Kuo, Nuyens (2016).

Typical QMC finite element error analysis

Denote by $u_h^s(\boldsymbol{x}, \boldsymbol{y}) := u_h(\boldsymbol{x}, (\boldsymbol{y}_{\{1:s\}}; 0))$ the FE approximation of a weak solution of the PDE with truncated diffusion coefficient $a(\boldsymbol{x}, (\boldsymbol{y}_{\{1:s\}}; 0))$, where u_h is a FE approx. and we set $(\boldsymbol{y}_{\{1:s\}}; 0) = (y_1, \ldots, y_s, 0, 0, \ldots)$.

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The mean square error can be bounded by

$$\mathbb{E}_{\boldsymbol{\Delta}}\left[\left|\mathbb{E}[G(u)] - Q_N(G(u_h^s), \boldsymbol{z}, \boldsymbol{\Delta})\right|^2\right] \leq \mathbb{E}_{\boldsymbol{\Delta}}\Big[\big(\underbrace{I_s(G(u_h^s)) - Q_N(G(u_h^s), \boldsymbol{z}, \boldsymbol{\Delta})}_{\text{QMC integration error}}\big)^2\Big]$$

$$+ 2\big(\underbrace{\mathbb{E}[G(u)] - I_s(G(u^s))}_{\text{dimension truncation error}}\big)^2 + 2\big(\underbrace{I_s(G(u^s)) - I_s(G(u_h^s))}_{\text{finite element error}}\big)^2$$

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- Estimates for dimension truncation and finite element error known
- QMC error contribution can be bounded (using known error bounds for CBC-type constructions)

Quality measure and function space

Worst-case error

For a Banach space $(\mathcal{F}, \|\cdot\|_{\mathcal{F}})$ and a QMC rule Q_N with point set $P_N = \{\boldsymbol{y}_1, \ldots, \boldsymbol{y}_N\} \subset [0,1]^s$ the *worst-case error* is defined as

$$e_{N,s}(Q_N, \mathcal{F}) := \sup_{\|F\|_{\mathcal{F}} \le 1} \left| \int_{[0,1]^s} F(\boldsymbol{y}) \, \mathrm{d}\boldsymbol{y} - \frac{1}{N} \sum_{k=1}^{N} F(\boldsymbol{y}_k) \right|.$$

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Function space setting: Weighted, unanchored Sobolev space $\mathcal{W}_{s,\boldsymbol{\gamma}}$ defined over $[-\frac{1}{2}, \frac{1}{2}]^s$ with square integrable mixed first derivatives and non-negative weights $\boldsymbol{\gamma} = (\gamma_{\mathfrak{u}})_{\mathfrak{u} \subseteq \{1:s\}}$. The norm for $F \in \mathcal{W}_{s,\boldsymbol{\gamma}}$ equals

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- We will consider lattice rules, a special family of QMC rules:

Definition: Rank-1 lattice rule

A *rank-1 lattice rule* is a quasi-Monte Carlo method of the form

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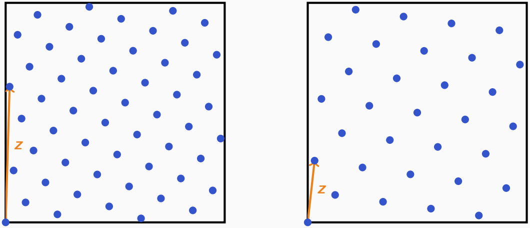

Figure 2: Fibonacci lattice with $N = 55$ and $\boldsymbol{z} = (1, 34)$ (left) and a rank-1 lattice with $N = 32$ and $\boldsymbol{z} = (1, 9)$ constructed by the CBC construction (right)

QMC integration error contribution

- Regularity analysis reveals that derivative bounds of POD form, i.e.,

$$\|\partial^{\boldsymbol{\nu}} u(\cdot, \boldsymbol{y})\|_V \leq C\, \boldsymbol{b}^{\boldsymbol{\nu}}\, \Gamma(|\boldsymbol{\nu}|)\, \|f\|_{V^*}.$$

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with constant

$$C_{\boldsymbol{\gamma},\lambda} := \Big[\sum_{\emptyset\neq\mathfrak{u}\subseteq\{1:s\}} \gamma_{\mathfrak{u}}^{\lambda}\, \varrho^{|\mathfrak{u}|}(\lambda) \Big]^{\frac{1}{\lambda}} \Big[\sum_{\mathfrak{u}\subseteq\{1:s\}} \frac{\Gamma(|\mathfrak{u}|)^2 \prod_{j\in\mathfrak{u}} b_j^2}{\gamma_{\mathfrak{u}}} \Big].$$

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- The resulting weights $\gamma_{\mathfrak{u}}^*$ which minimize the constant $C_{\boldsymbol{\gamma},\lambda}$ are therefore also of POD form and depend on the random field $a(\boldsymbol{x},\boldsymbol{y})$.

Motivation

- Seminal article by Kuo, Schwab, Sloan (2012) on QMC FEM for elliptic PDEs with random coefficients showed that the occurring weights are of POD form, i.e., $\gamma_{\mathfrak{u}} = \Gamma(|\mathfrak{u}|) \prod_{j \in \mathfrak{u}} \gamma_j$

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- **Problem 2:** Currently, the lattice rules have to be computed for every individual problem (depending on $a(\boldsymbol{x}, \boldsymbol{y})$) leading to high computational efforts when many problems are solved.

Open Problem

Problem

- Device QMC finite element methods for the given PDE class that can be used simultaneously for a range of problems (without needing to construct a QMC rule repeatedly)
- Show theoretically and numerically that such methods achieve good error convergence rates

Subproblems:

- Either: Device new QMC/lattice rules which yield almost optimal error convergence rates for a large range of weight sequences
- Or: Show that existing constructions can achieve this goal provided that the weight sequences satisfy certain conditions

Thank you for your attention!